Ground state of an impurity in a quasi-two-dimensional Fermi gas

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We study the ground state of a highly imbalanced Fermi gas under quasi-two-dimensional confinement. We find that for typical experimental conditions, the location of the recently predicted polaron-molecule transition is shifted to lower values of the vacuum binding energy due to the interplay between transverse confinement and many-body physics. The energy of the attractive polaron is calculated in the 2D-3D crossover and displays a series of cusps before converging towards the 3D limit.

Understanding the many-body properties of two-dimensional (2D) cold atomic Fermi gases may provide insight into puzzling condensed matter systems, such as exotic pairing in heavy fermion materials, quasi-2D organic superconductors, and thin film superconductors [1–3]. What these systems have in common is that they display intriguing behavior when pairing of electrons in opposite spin states is frustrated by strong Zeeman magnetic fields, effectively causing an imbalance between spin-↑ and ↓ fermions. In this Letter we study the analogous problem of the highly polarized limit of a quasi-2D Fermi gas.

Recently, several experimental groups have realized quasi-2D Fermi gases with ultra-cold atoms [4–10]. In these experiments a three-dimensional (3D) Fermi gas is confined into a single layer (or a stack of layers) by a tight transverse harmonic oscillator potential $V(z) = \frac{1}{2}m\omega_z^2 z^2$. If the temperature T and Fermi energy $\epsilon_F = \hbar^2 k_F^2/2m$, where k_F is the Fermi wave vector and m is the atomic mass, satisfy $k_B T \ll \epsilon_F \ll \hbar\omega_z$ the gas is quantum degenerate and collisions can be considered to be quasi-2D as transverse degrees of motion are frozen out [11].

We consider the highly population imbalanced limit of a single spin-↓ impurity in a Fermi sea of spin-↑ atoms. In this limit, it was predicted that the Fermi sea can destroy pairing (if interactions are sufficiently weak) and give rise to a Fermi polaron [12, 13], an impurity dressed by excitations of the Fermi sea, in addition to the molecular state appearing at stronger coupling. From a dimensional analysis of the quasi-2D Fermi gas, the location of the polaron-molecule transition should depend on ϵ_B/ϵ_F and an additional parameter describing the quasi-2D confinement (i.e. $\epsilon_F/\hbar\omega_z$). This is to be contrasted with the previously studied case of infinitely tight 2D trapping [14], whose properties depend solely on the dimensionless interaction parameter ϵ_B/ϵ_F. As shown in Fig. 1, we find that the value of ϵ_B/ϵ_F where this transition occurs strongly depends on the value of $\epsilon_F/\hbar\omega_z$. The transition is shifted to lower ϵ_B/ϵ_F at higher densities, in good agreement with the experimental measurement of Ref. [10]. The 2D limit considered in Ref. [14] is recovered as $\epsilon_F/\hbar\omega_z \to 0$. The 2D description breaks down as the size of molecules (or polarons) approaches the harmonic oscillator length of the transverse confine-
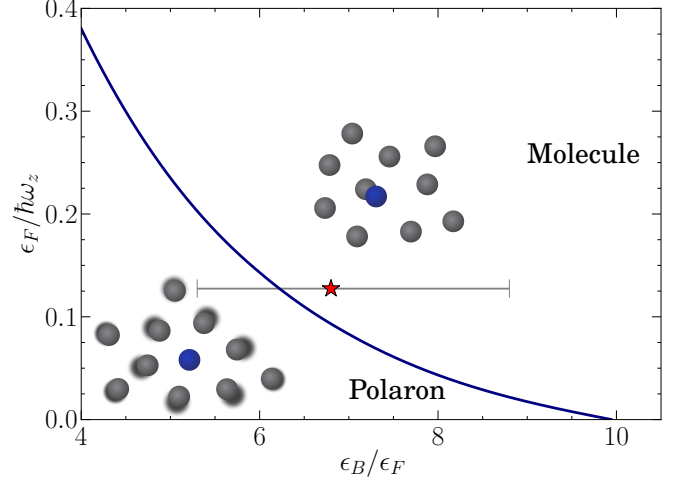

FIG. 1: (color online). Phase diagram of a highly polarized quasi-two dimensional Fermi gas. Below the line, the single spin-↓ impurity exists as a polaron dressed by the Fermi sea of spin-↑ atoms. For large binding energies, the impurity forms a molecular bound-state. The location of the transition depends on the strength of the external confinement: At higher density (or weaker confinement) the transition occurs at lower ϵ_B/ϵ_F. The result from the recent experiment by Koschorreck *et al.* [10] is also shown (star).

ment $l_z = \sqrt{\hbar/m\omega_z}$.

We also demonstrate how this quasi-2D physics is manifested in the energy of the repulsive polaron of the quasi-2D upper branch gas [15, 16]. As we will argue, in the repulsive branch, a single effective interaction parameter describing quasi-2D collisions provides a sufficient description as long as the (non-universal) lifetime of the repulsive polaron is large.

Finally, we present results for the energy of an impurity in the dimensional crossover regime from quasi-2D to 3D, where $\epsilon_F \gtrsim \hbar\omega_z$. This regime was studied experimentally in Ref. [6], and also very recently in Ref. [9] where features in RF-spectra were interpreted as transitions between polaronic states. The energy is found to exhibit an intriguing behavior, as it has a cusp each time the chemical potential of spin-↑ particles admits an extra harmonic oscillator level. Additionally, the energy is found to quickly approach the 3D limit.

The low energy scattering of two particles in a two-dimensional geometry is described through the s-wave scattering amplitude [17]

$$f(q) = \frac{2\pi}{\ln\left[1/(qa_{2D})\right] + i\pi/2}, \quad (1)$$

with q the relative momentum. In the following we work in units where $\hbar = 1$. The scattering at low energies is controlled by the parameter a_{2D} which has the dimension of length. a_{2D} may be extracted in experiments from the low energy behavior of the scattering cross section $\sigma = |f(q)|^2/4q$.

Petrov *et al.* [11] demonstrated how the scattering amplitude in a quasi-2D geometry is related to Eq. (1): In three dimensions, the properties of an atomic gas interacting close to a broad Feshbach resonance is characterized by a single few-body parameter, the scattering length a_s. The energy dependence of the quasi-2D scattering amplitude f_{00} at energy $\epsilon = k^2/m < \omega_z$ was found to be

$$f_{00}(\epsilon) = \frac{2\sqrt{2\pi}}{l_z/a_s - \mathcal{F}(-\epsilon/\omega_z)}, \quad (2)$$

where incoming and outgoing particles are assumed to be in the ground state of the relative motion in the harmonic oscillator potential. We use the definition of $\mathcal{F}$ [18]

$$\mathcal{F}(x) = \int_0^\infty \frac{du}{\sqrt{4\pi u^3}} \left(1 - \frac{e^{-xu}}{\sqrt{[1 - \exp(-2u)]/2u}}\right). \quad (3)$$

As opposed to scattering in 3D, the two-dimensional scattering always admits a bound state, whose binding energy $\epsilon_B > 0$ satisfies $l_z/a_s = \mathcal{F}(\epsilon_B/\omega_z)$. At low energies, $|\epsilon| \ll \omega_z$, the function $\mathcal{F}$ takes the form

$$\mathcal{F}(x) \approx \frac{1}{\sqrt{2\pi}} \ln\left(Bx/\pi\right) + \frac{\ln 2}{\sqrt{2\pi}} x + \mathcal{O}(x^2) \quad (4)$$

with $B \approx 0.905$ [11, 18]. Keeping the first term on the r.h.s., the asymptotic low energy expression (1) is recovered with

$$a_{2D} = l_z\sqrt{\pi/B}\exp(-\sqrt{\pi/2}l_z/a_s). \quad (5)$$

As demonstrated below, going beyond the leading order in the low energy expansion of $\mathcal{F}(x)$ is important for the understanding of current experiments on Fermi gases confined to quasi-2D.

We now turn the problem of a single $\downarrow$ impurity in a Fermi sea of $\uparrow$ particles. A central tool in the study of many-body problems is the T-matrix, describing the forward scattering between the impurity and a spin-$\uparrow$ atom at total 2D momentum $\mathbf{q}$ and energy ϵ. In vacuum, the T-matrix is simply related to the scattering amplitude

$$\mathcal{T}_0(\mathbf{q}, \epsilon) = f_{00}(\epsilon - \epsilon_{\mathbf{q}}/2)/m, \quad (6)$$
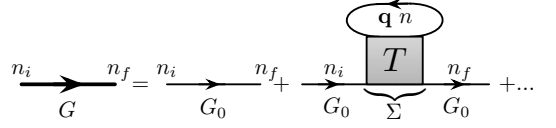

FIG. 2: The first two terms of the geometric series for the propagator of the impurity dressed by a particle-hole excitation.

with the free particle dispersion $\epsilon_{\mathbf{q}} = q^2/2m$. The presence of the Fermi sea couples the center of mass and relative harmonic oscillator modes and the T-matrix depends on harmonic oscillator quantum numbers n_1, n_2 and n_1', n_2' of incoming and outgoing particles. The formalism for the T-matrix in the presence of the Fermi sea was recently developed in Ref. [19] where it was demonstrated that the full T matrix, $T_{n_1'n_2'}^{n_1 n_2}$, can be written in terms of a T-matrix depending only on center of mass quantum numbers N, N'. For details see Ref. [19] and the Supplementary material.

In the limit of weak attractive interactions, the impurity exists as a quasi-particle dressed by a cloud of majority atoms. This impurity problem has been widely studied theoretically in both three [12, 20] and two dimensions [14–16, 21, 22] using variational and diagrammatic methods. In 3D, the accuracy of this analytic approach has been validated by both exact quantum Monte-Carlo calculations [23], and also by precise experiments with quantum simulators employing optically trapped ultracold quantum gases [24]. Here we provide an extension of the diagrammatic approach to the experimentally relevant quasi-2D setting.

Consider the propagation of the impurity, initially in the state of harmonic oscillator quantum number n_i. Interactions with a particle from the majority Fermi sea may change the state into a final state with quantum number n_f. Conservation of parity further restricts $n_i - n_f$ to be even. In the single particle-hole approximation, the propagator of the impurity then takes the form of a matrix equation

$$G(\mathbf{p}, \epsilon) = \left[G_0^{-1}(\mathbf{p}, \epsilon) - \Sigma(\mathbf{p}, \epsilon)\right]^{-1}, \quad (7)$$

obtained by summing the geometric series illustrated in Fig. 2. Note that the diagrams are formally identical to those considered in 3D [20], however each propagator is now assigned a harmonic oscillator quantum number which is summed over intermediate states. The bare propagator is given by the diagonal matrix $G_0^{nn'}(\mathbf{p}, \epsilon) = \delta_{nn'}/\left[\epsilon - \epsilon_{\mathbf{p}n} + i0\right]$ and the self energy is

$$\Sigma_{n_1 n_2}(\mathbf{p}, \epsilon) = \sum_{\mathbf{q}, n} T_{n_2 n}^{n_1 n}(\mathbf{p} + \mathbf{q}, \epsilon + \epsilon_{\mathbf{q}n})\, n_{F\uparrow}(\mathbf{q}, n), \quad (8)$$

where $\epsilon_{\mathbf{p}n} \equiv \epsilon_{\mathbf{p}} + n\omega_z$. The Fermi function n_F takes the value 1 if the state with momentum $\mathbf{q}$ and harmonic oscillator quantum number n is occupied in the $\uparrow$ Fermi
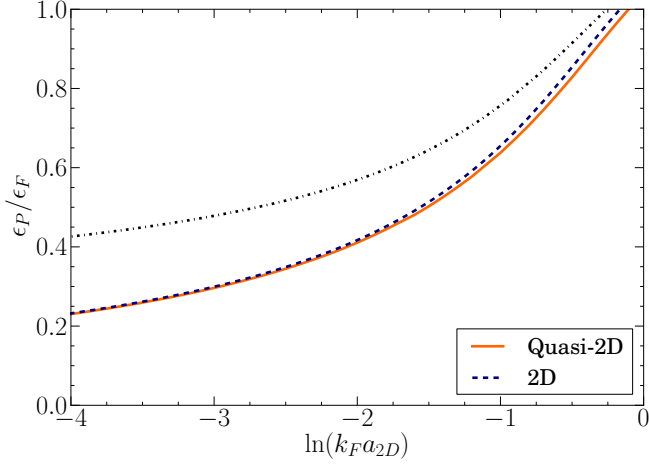
FIG. 3: (color online). Energy ϵ_P/ϵ_F of an impurity interacting repulsively with a Fermi sea as a function of interaction strength. The energy of a quasi-2D impurity is shown for $\epsilon_F/\omega_z = 0.1$ (solid line). Additionally we show the 2D results of Ref. [16] using the often used assumption $a_{2D} = 1/\sqrt{m\epsilon_B}$ (dotted), and also using Eq. (1) as definition of a_{2D} (dashed).
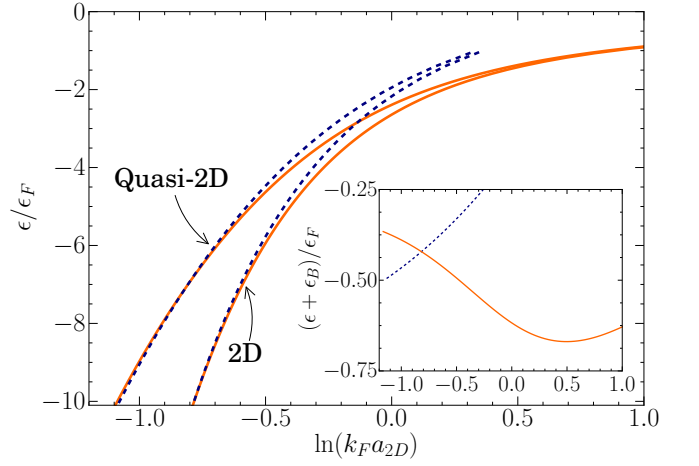

FIG. 4: (color online). Energy of the attractive polaron (solid line) and molecule (dashed) in the 2D regime and in quasi-2D ($\epsilon_F/\omega_z = 1/10$). The molecule energy has been shifted by ϵ_F to reflect that a particle has been removed from the Fermi sea. The inset shows the quasi-2D energies of the main figure with the binding energy subtracted.

sea, and zero otherwise. The energy of the polaron corresponds to a pole of $G(\mathbf{p}, \epsilon)$. From Eq. (7) the energies of both the attractive and the repulsive polaron may then be obtained.

The energy of the repulsive polaron as a function of interaction strength is shown in Fig. 3. As opposed to the attractive polaron, our calculation demonstrates that the energy of the repulsive polaron depends solely on the interaction parameter $k_F a_{2D}$. This is to be expected as $|\epsilon_P| \ll \omega_z$ and thus the energy should match previous studies of the repulsive polaron in 2D [15, 16]. Furthermore, Fig. 3 demonstrates that in order to compare the predictions of these 2D theories to experiments with quasi-2D Fermi gases, one should not match the binding energy of the 2D theory to that of the quasi-2D system. Instead the 2D scattering length a_{2D} defined in (1) and calculated by using the low energy quasi-2D scattering amplitude in Eqs. (2)-(5) should be used. Note that while the energy of the repulsive polaron depends solely on $k_F a_{2D}$, the decay rate depends sensitively on the energy difference between the repulsive polaron and the lower lying states [25] and is thus non-universal.

As the strength of interactions is increased, the impurity binds a particle from the Fermi sea to form a molecule. As in the case of the polaron state, the molecule is in turn dressed by particle-hole pairs. The molecule dressed by one particle-hole pair has been studied in 3D [26–28] and in 2D [14] by variational and diagrammatic methods. Here we extend the diagrammatic method of Combescot et al. [26] to include harmonic confinement. To this end, we note that the confinement does not change the structure of the diagrams needed for the molecule energy. The difference in the present

problem is that all fermion propagators are assigned a harmonic oscillator quantum number and the T-matrix depends on these. Assuming $\epsilon_F < \omega_z$ such that in the non-interacting Fermi gas only the ground state of the harmonic oscillator potential is occupied, the energy of the dressed molecule is obtained when the equation

$$H_{\mathbf{qk}}^{n_1 n_2 n_3} = \sum_{n_1' n_2'} T_{n_1' n_2'}^{n_1 n_2}(\mathbf{q} - \mathbf{k}, \epsilon + \epsilon_{\mathbf{q}0} - \epsilon_{\mathbf{k}n_3})[1 - n_{F\uparrow}(\mathbf{k}, n_3)]$$

$$\times \left\{ \sum_{\mathbf{k}'} \frac{H_{\mathbf{qk}'}^{n_3 n_2' n_1'}}{E_{\mathbf{kk'q}}^{n_1' + n_2' + n_3}} [1 - n_{F\uparrow}(\mathbf{k}', n_1')] - \delta_{0n_1'} \sum_{\mathbf{q}'} \frac{H_{\mathbf{q'k}}^{0n_2' n_3}}{E_{\mathbf{k}}^{n_2' + n_3}} \right.$$

$$\left. + \delta_{0n_1'} \sum_{n_2'' n_3'} \frac{T_{n_2'' n_3'}^{n_2' n_3}(\mathbf{0}, \epsilon)}{E_{\mathbf{k}}^{n_2' + n_3}} \sum_{\mathbf{q'k'}} \frac{H_{\mathbf{q'k'}}^{0n_2'' n_3'}}{E_{\mathbf{k'}}^{n_2'' + n_3'}} [1 - n_{F\uparrow}(\mathbf{k}', n_3')] \right\} \quad (9)$$

has a solution. The vertex H includes all diagrams occurring in atom-dimer scattering in a quasi-2D geometry [29]. The sum on $\mathbf{q}'$ is up to k_F while the sum on $\mathbf{k}'$ is over all possible momenta. We use the notations $E_{\mathbf{k}}^n \equiv -\epsilon + \epsilon_{\mathbf{k}} + n\omega_z$ and $E_{\mathbf{kk'q}}^n \equiv -\epsilon - \epsilon_{\mathbf{q}} + \epsilon_{\mathbf{k}} + \epsilon_{\mathbf{k}'} + \epsilon_{\mathbf{k}+\mathbf{k}'-\mathbf{q}} + n\omega_z$. For further details see the Supplementary material.

In Fig. 4 we display the energy of the attractive polaron and the molecule in the 2D limit and in quasi-2D. As may be seen, the polaron and molecule energies cross at a very small angle and thus the position of the polaron-molecule transition depends sensitively on the confinement. Computing the position of the polaron-molecule transition as a function of the strength of confinement, ϵ_F/ω_z, yields the phase diagram in Fig. 1. As the confinement is weakened from the 2D limit (or the density increased), the transition is seen to move towards smaller ϵ_B/ϵ_F. In particular, in the experiment of Ref. [10] with
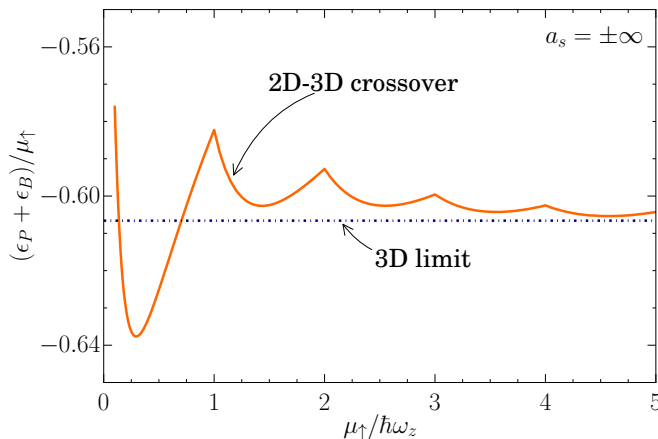
FIG. 5: (color online). The energy of the attractive polaron in quasi-2D on the 3D Feshbach resonance. The dotted line is the 3D limit $\epsilon_P = -0.6066\mu_\uparrow$ [12, 20].

parameters $\omega_z = 2\pi \times 78.5$ kHz and $\epsilon_F = 2\pi \times 10$ kHz the transition was found at $\epsilon_B/\epsilon_F \approx 6.8$ while our theory predicts the transition to occur at $\epsilon_B/\epsilon_F \approx 6.2$ (see Fig. 1). This should be contrasted with the 2D prediction of $\epsilon_B/\epsilon_F \approx 10$ at the polaron molecule transition [14].

Our formalism is also useful for studying the dimensional crossover from 2D to 3D in polarized Fermi gases. To illustrate this, we consider the energy of the attractive polaron on the 3D Feshbach resonance, where the binding energy of the weakly bound dimer takes the universal value $\epsilon_B = 0.244\omega_z$ [18]. Our results are shown in Fig. 5. Spin-$\uparrow$ atoms in the n-th excited harmonic oscillator level become available whenever the chemical potential $\mu_\uparrow \geq n\omega_z$. The polaron energy is seen to develop a cusp each time a new state becomes available due to the increase in the density of $\uparrow$ states. The polaron energy is seen to rapidly approach the 3D limit of an impurity dressed by one particle-hole pair.

We remark on the resemblance between the above approach and the study of the ground state of a spin polarized 3D Fermi gas near a narrow Feshbach resonance [24, 30, 31]. The narrowness is due to a large effective range which enters the problem in addition to the scattering length and the Fermi wave vector. For fixed scattering length, an increase in the effective range leads to weaker interactions and a smaller binding energy. In the quasi-2D problem, the length-scale l_z plays the role of an effective range: Indeed, similarly to our results in Fig. 1 for increased l_z, Refs. [24, 30, 31] found the polaron-molecule transition to be shifted towards smaller binding energies for increased effective range in 3D.

To conclude, we have provided a theory for the highly imbalanced Fermi gas in quasi-2D. Experimentally, the phase diagram Fig. 1 may be mapped out by varying the strength of the harmonic confinement ω_z or the density in an ultra-cold quasi-2D Fermi gas. Upon entering the molecular phase, the quasi-particle residue of the impu-

rity abruptly drops to zero [27], which leaves a clear signature in the line-shape of RF-spectra [10, 13, 24]. Similarly, the energy of impurities in ultra-cold Fermi gases have been extracted in quasi-2D from ARPES spectra, obtained via momentum resolved RF-spectra [10].

Finally, we point out that while we considered the experimentally more relevant quasi-2D problem, our results are also of relevance to the analogous problem of quasi-1D Fermi gases [32–35]. For example, similar to our results for the quasi-2D Fermi gas, one expects that the phase diagram of the 1D imbalanced gas provides an inadequate description at stronger coupling.

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Supplementary material

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T-matrix in the medium

Consider the scattering of two particles at 2D momentum $\mathbf{q}$ and energy ϵ. The T-matrix describing forward scattering in the medium in the presence of harmonic confinement was recently calculated in Ref. [19], we include it here for completeness: For incoming and outgoing harmonic oscillator quantum numbers n_1, n_2 and n_1', n_2', the T-matrix describing forward scattering in the medium takes the form

$$T_{n_1'n_2'}^{n_1 n_2}(\mathbf{q}, \epsilon) = \sqrt{2\pi} l_z \sum_{NN'n_r n_r'} C_{Nn_r}^{n_1 n_2} C_{N'n_r'}^{n_1'n_2'} \phi_{n_r}^*(0) \phi_{n_r'}(0) \mathcal{T}_{N,N'}(\mathbf{q}, \epsilon), \tag{10}$$

in terms of relative and center of mass quantum numbers n_r, n_r' and N, N'. The Clebsch-Gordan coefficients for the change of basis are given by [36]

$$C_{Nn_r}^{n_1 n_2} = 2^{-\frac{1}{2}(n_1+n_2)} \sqrt{\frac{N!n_r!}{n_1!n_2!}} \sum_{m=\max(n_r-n_1,0)}^{\min(n_r,n_2)} (-1)^m \binom{n_1}{n_r-m} \binom{n_2}{m}, \tag{11}$$

and the harmonic oscillator wavefunction ϕ takes the value

$$\sqrt{2\pi} l_z |\phi_n(0)|^2 = \begin{cases} \frac{(n-1)!!}{n!}, & \text{n even} \\ 0 & \text{n odd} \end{cases} \tag{12}$$

at the origin. $\mathcal{T}_{NN'}$ is renormalized by the use of the two-body T-matrix as [19]

$$\mathcal{T}_{NN'}^{-1}(\mathbf{q}, \epsilon) = \mathcal{T}_0^{-1}(\epsilon - N\omega_z - \epsilon_\mathbf{q}/2)\delta_{NN'} - \mathcal{D}_{NN'}(\mathbf{q}, \epsilon), \tag{13}$$

with the renormalized polarization operator given by

$$\mathcal{D}_{NN'}(\mathbf{q}, \epsilon) = -\sum_{n_1 n_2 \mathbf{k}} u_{n_1+n_2-N, n_1+n_2-N'} C_{N', n_1+n_2-N'}^{n_1 n_2} C_{N, n_1+n_2-N}^{n_1 n_2} \frac{n_{F\uparrow}(\mathbf{q}-\mathbf{k}, n_1) + n_{F\downarrow}(\mathbf{k}, n_2)}{\epsilon - \epsilon_{\mathbf{q}-\mathbf{k}} - \epsilon_\mathbf{k} - \omega_z(n_1+n_2)} \tag{14}$$

and expansion coefficients $u_{n,m} = (-1)^{(n+m)/2}(n-1)!!(m-1)!!/\sqrt{n!m!}$ for n, m even non-negative integers, 0 otherwise. The Fermi function $n_{F\uparrow}(\mathbf{k}, n_1)$ is 1 for a particle in the $\uparrow$ Fermi sea, 0 otherwise. For the polarized gas considered in this Letter, the Fermi function $n_{F\downarrow}(\mathbf{k}, n_2)$ vanishes.

Equation for the dressed molecule

We now construct the sum of diagrams needed to obtain the energy of the molecular state dressed by one particle-hole pair in the presence of harmonic confinement. Formally, the diagrams are identical to those considered in Ref. [26] for the 3D problem, although in the present problem all fermion lines have additional harmonic oscillator quantum numbers. For simplicity, we restrict ourselves to a molecule at rest. We also require $\epsilon_F < \omega_z$ such that hole propagation always proceeds in the lowest harmonic oscillator state. Our results are easily generalizable to finite momentum and occupation of higher bands.

The bound state energy corresponds to a divergence of a two-particle vertex. As argued in Ref. [26], the energy of the molecule dressed by one particle-hole pair necessarily lies below the energy of the bare molecule. Thus it suffices to consider the vertex H describing the sum of diagrams containing a maximum of two forward propagating $\uparrow$ atoms as well as the impurity atom. The integral equation satisfied by H is depicted in Fig. 6: In the vertex H the initial interaction is between the impurity and the $\uparrow$ atom with quantum number n_1. After this interaction, this particle either closes its own loop (the last two diagrams on the r.h.s. of Fig. 6) or participates in another vertex
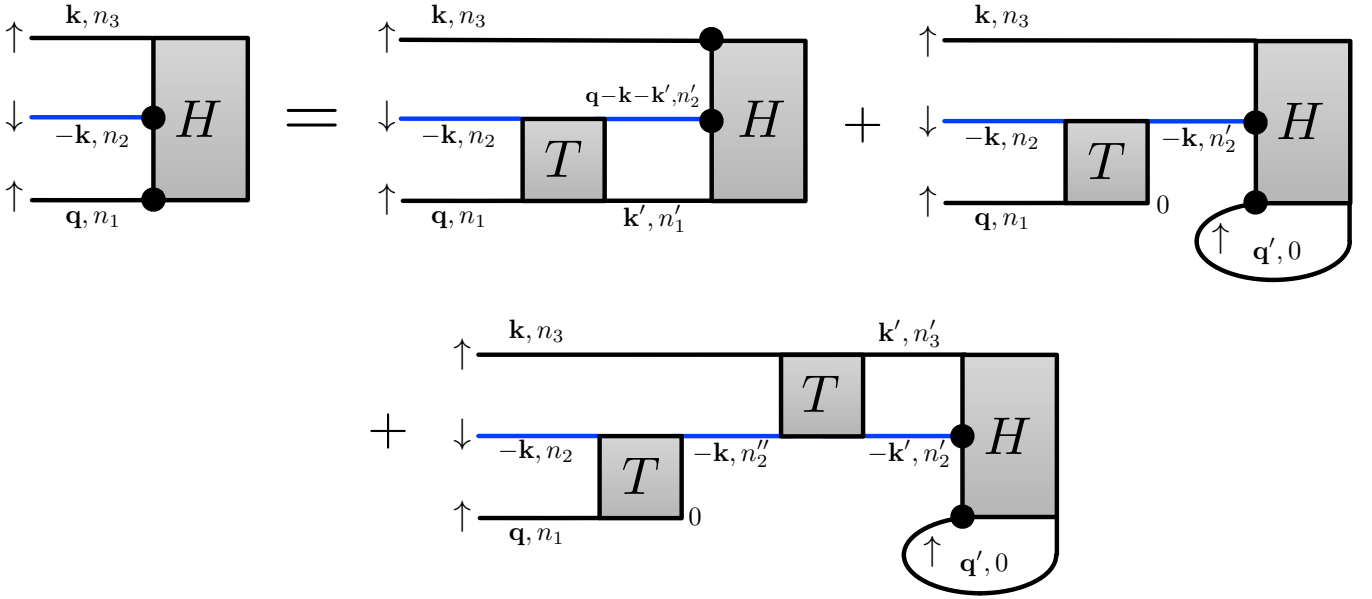
FIG. 6: (color online). The integral equation (9) satisfied by the vertex H. Circles indicate that the interaction inside the vertex is initially between the two marked particles. The loop on the last two diagrams yields a summation over $\mathbf{q}'$.

H. Taking into account only the homogenous terms (any pole in the non-homogenous term lies above the dressed molecule energy) finally results in the integral equation (9) in the main text.

Additionally, we have verified that a variational approach with the trial wave functions for the polaron

$$|P\rangle = \sum_n \phi_n c_{\downarrow \mathbf{0}n}^\dagger |\text{FS}, N_\uparrow\rangle + \sum_{\substack{nn'm \\ \mathbf{kq}}} \phi_{\mathbf{kq}}^{nn'm} c_{\downarrow \mathbf{q}-\mathbf{k}n}^\dagger c_{\uparrow n'\mathbf{k}}^\dagger c_{\uparrow m\mathbf{q}} |\text{FS}, N_\uparrow\rangle \tag{15}$$

and the molecule

$$|M\rangle = \sum_{nn'\mathbf{k}} \phi_k^{nn'} c_{\uparrow \mathbf{k}n}^\dagger c_{\downarrow -\mathbf{k}n'}^\dagger |\text{FS}, N_\uparrow - 1\rangle + \frac{1}{2} \sum_{\substack{nn'mm' \\ \mathbf{kk'q}}} \phi_{\mathbf{kk'q}}^{nn'mm'} c_{\downarrow \mathbf{q}-\mathbf{k}-\mathbf{k}'n}^\dagger c_{\uparrow \mathbf{k}n'}^\dagger c_{\uparrow \mathbf{k}'m}^\dagger c_{\uparrow \mathbf{q}m'} |\text{FS}, N_\uparrow - 1\rangle \tag{16}$$

yields the equations (7) for the polaron and (9) for the molecule quoted in the main text. Here $c_{\sigma \mathbf{k}n}^\dagger$ denotes the creation operator for a particle of spin σ with in-plane momentum $\mathbf{k}$ in the n-th transverse harmonic oscillator mode. $|\text{FS}, N_\uparrow\rangle$ is the non-interacting ground-state of $N_\uparrow$ spin-$\uparrow$ fermions.